Impact of CO_2 Mixing with Trapped Hydrocarbons on CO_2 Storage Capacity and Security: A Case Study from the Captain Aquifer (North Sea)

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Abstract

Gas mixing in the subsurface could have crucial implications on CO_2 storage capacity and security. This study illustrates the impact of gas mixing in the "Captain X" CO_2 storage site, an open saline aquifer and subset of the greater Captain aquifer, located in the Moray Firth, North Sea. The storage site hosts several abandoned hydrocarbon fields where injected CO_2 could interact and mix with any remaining hydrocarbon gas left in the depleted structures. For this study, compositional simulation of CO_2 injection into the Captain X storage site reservoir model was conducted to quantify the impact of mixing. Results show mixing of CO_2 with the remaining trapped hydrocarbon gas makes the plume considerably less dense and more mobile. This increases the buoyancy forces acting on the plume, causing it to migrate faster towards the shallower storage boundaries and therefore, reduces the storage capacity of the site. Mixing also compromises the storage security as it mobilises the structurally trapped hydrocarbon gas from within the abandoned fields. Informed injector placement helps to manage and reduce the impact of mixing. Correct assessment of mixing is also considerably dependent on the volume and property of the trapped hydrocarbon gas. To provide a correct long term understanding of storage capacity and security, the impact of mixing, therefore, needs to be correctly considered in all large-scale CO_2 storage operations.

Keywords: CCUS, CO_2 Storage, Mixing, Saline Aquifer, Plume Migration, Compositional Modelling

1. Introduction

Despite continued development of renewable energy sources, fossil fuels are expected to remain a key source of energy for the foreseeable future [1,2]. Burning of fossil fuels, however, generates large volumes of greenhouse CO_2 which contributes significantly to global warming and climate change. Subsurface storage of CO_2 has been proposed as a suitable mitigation strategy to stop the rising levels of CO_2 in the atmosphere in near future. CO_2 can be injected subsurface under different development configurations; either for pure storage or for enhanced oil recovery, where the incentives from oil may outstrip that from CO_2 tax [3].

As with many countries, the United Kingdom is committed to reduce its net global greenhouse gas emission to zero by the year 2050 [4]. One effective and secure strategy to mitigate CO_2 emissions is the geological storage of CO_2 in saline aquifers located in the United Kingdom Continental Shelf (UKCS) [5,6]. Saline aquifers, located in sedimentary basins all over the world, are excellent targets for CO_2 storage as they offer considerably larger storage capacities than many other settings [7].

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Various saline aquifers have been identified in the North Sea Basin around the UKCS and have been studied for the purpose of CO_2 storage [8,9]. These include some of the Bunter sandstone closures in the Southern North Sea [10,11], the Forties sandstone of the Forties aquifer [12] and the Captain aquifer in the Central North Sea [13].

Containment and security of storage are important considerations for choosing the most suitable CO_2 storage site. These factors mandate that the stored CO_2 must be contained within the storage site during initial injection to well after injection cessation. In terms of containment, saline aquifers can be classified into two categories of "open" and "closed" aquifer systems [14]. Closed aquifers are those in which the fluids in the system e.g. brine, hydrocarbons or CO_2 are primarily "structurally" contained. For CO_2 storage, this means the injected CO_2 remains immobile post injection due to the presence of physical closures such as faults, pinch-outs or dome-shaped structures that prohibits CO_2 migration.

In open saline aquifers, however, there are no physical barriers to structurally immobilise CO_2 and the plume is expected to be immobilised by other trapping mechanisms, mainly solubility and residual trapping. Once injection stops in these systems, the CO_2 plume may migrate under the influence of buoyancy forces [15] and the characteristics of this migration determine the maximum storage capacity in these aquifers. The faster the plume migration, there is less opportunity for CO_2 to be immobilised via solubility and residual trappings, and thus the risk for CO_2 to cross the predefined set storage boundary is increased. A remedy for this is a reduction of the injected CO_2 inventory, i.e. the final storage capacity of the site, in order to allow the trapping mechanisms to immobilise the plume before storage boundaries are crossed [12]. The non-geological license boundaries in open aquifer storage systems are often selected based on detailed engineering considerations, such as to limit the interaction between various immediately adjacent storage sites, or to minimise interaction between the CO_2 storage site and nearby petroleum activities and any other subsurface users in general [13]. In such systems, storage development design involves modelling of CO_2 storage for few hundreds to even thousands years after injection cessation to provide assurance regarding the permanent containment of CO_2 and its security of storage [16].

The degree of buoyancy driven plume migration in open saline aquifers is a function of vertical permeability, the structural tilt of the storage site and importantly, the density contrast between plume and the resident brine. The larger any of these parameters, the greater the significance of the buoyancy forces acting on the plume, resulting in faster migration which ultimately reduces the final storage capacity.

As open aquifers are usually very extensive structures, they may host several hydrocarbon fields at various stages of developments. In fact, the presence of hydrocarbon systems within a saline aquifer indicates the existence of a promising caprock that has provided an effective seal for the hydrocarbons for millions of years, and therefore, provides good prospect for the vertical containment of the injected CO_2. Plume migration in such open aquifers, with hosted hydrocarbon systems may cause the injected CO_2 to come into contact and interact with non-CO_2 resident fluids, usually of lighter density left in these hydrocarbon-filled structures. This can unexpectedly reduce the plume density affecting the overall plume dynamics and thus, its migration characteristics. In this study we identify this interaction phenomenon as "mixing". The mixing of injected CO_2 and lighter *in-situ* hydrocarbon gas can take place wherever CO_2 storage meets hydrocarbons in the subsurface, a likely situation in future CCS developments as the presence of hydrocarbons is often regarded as a confirmation of suitable storage characteristics [17,18]. Worldwide examples include storage systems from the North Sea (Europe) [8], the Gulf of Mexico (US) [19,20] or the Middle East [21], all of which have been appraised for CO_2 storage activities.

This study illustrates the impact of mixing for CO_2 injection in Captain X storage site, an open aquifer storage system and part of the greater Captain aquifer located in the Moray Firth, North Sea, but it is relevant for most large scale storage operations in saline aquifers. The site has previously been appraised for CO_2 storage [22,23] as part of several studies and possesses characteristics that makes it a suitable prospect for CO_2 storage. This includes a high storage capacity, high injectivity, availability of infrastructure for CO_2 transportation and its proximity to the St. Fergus gas processing plant as a small early source of CO_2 supply [24]. We first review the theoretical concept of mixing, then a

description of the Captain X and Captain aquifer are presented, after which the results of the numerical modelling of CO_2 storage in the Captain X considering mixing will be presented and discussed. A final sensitivity analysis section illustrates the impact of major uncertainties affecting the mixing phenomenon.

2. The Theoretical Concept of Mixing

The impact of gas mixing in subsurface systems have been investigated for different subsurface gas storage applications [25] including, CO_2 and methane [26] and hydrogen systems [27].These studies however have not covered the scale of large CO_2 storage in saline aquifers and depleted gas fields. Mixing in this context refers to the occurrence of direct contact between injected and resident fluids within the storage site, usually with different properties which may alter plume properties, notably its density and thus, may affect the storage characteristics. Figure 1 shows the density profile of a binary CO_2-methane system as a function of methane fraction at ambient Captain X subsurface conditions (P=19.70 MPa and T=65 °C) [28]. The data are generated using PVTi software [29].

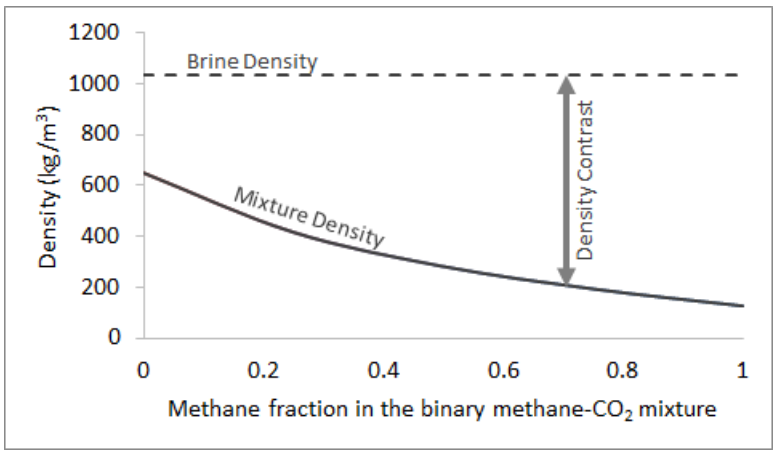

Figure 1: Theoretical concept of mixing. As methane concentration in the CO_2-methane mixture increases, mixture becomes lighter and its density contrast relative to aquifer brine increases.

Figure 1 shows that as the fraction of methane in the binary mixture increases, the mixture becomes progressively lighter and its density contrast relative to the host brine increases. According to these data, a 50% increase in the methane fraction in the mixture increases the density contrast by more than 90% compared to the scenario where the mixture was made of pure CO_2. This contrast increases by a factor of 130% as CO_2 is completely replaced by methane in the mixture.

Conceptually, similar phenomenon may occur in the storage site. Packets of lighter density hydrocarbon gases located in abandoned hydrocarbon fields within the storage site may contact and mix with the CO_2-rich plume. This decreases the density of the plume and consequently increases the density contrast between plume and aquifer brine. Such large density contrast promotes the buoyancy forces acting on the plume and may increase the plume migration velocity should storage occurs in open aquifer systems. This has implications on CO_2 storage characteristics as will be discussed in this study. We illustrate how such phenomenon affects storage capacity and security in Captain X as an exemplar open aquifer system.

3. "Captain Aquifer" and "Captain X Storage Site"

3.1. The Captain Aquifer

The Captain aquifer is massive saline aquifer located in the outer Moray Firth region of the Central North Sea and approximately 100 km north-east of the St. Fergus gas processing plant (Figure 2). The panhandle shaped saline aquifer stretches over 200 km from north-west to south-east covering an area of approximately 3438 km^2. The estimated CO_2 storage capacity of the Captain aquifer is between 358 MT and 2,495 MT [30] enabling the aquifer to potentially host multiple CO_2 storage sites [31]. No CO_2 has yet been injected in this aquifer, however, several studies including the CO_2 Multistore

project [6], the Scottish Carbon Capture and Storage (SCCS) report [32], recent geomechanical and petrographic assessment of the storage site [33] and the ETI-UKSAP project [9] have all identified the suitability of the Captain aquifer for CO_2 storage. Based on these studies, the Captain aquifer has been selected as the primary storage site for the Acorn CCS storage development [24].

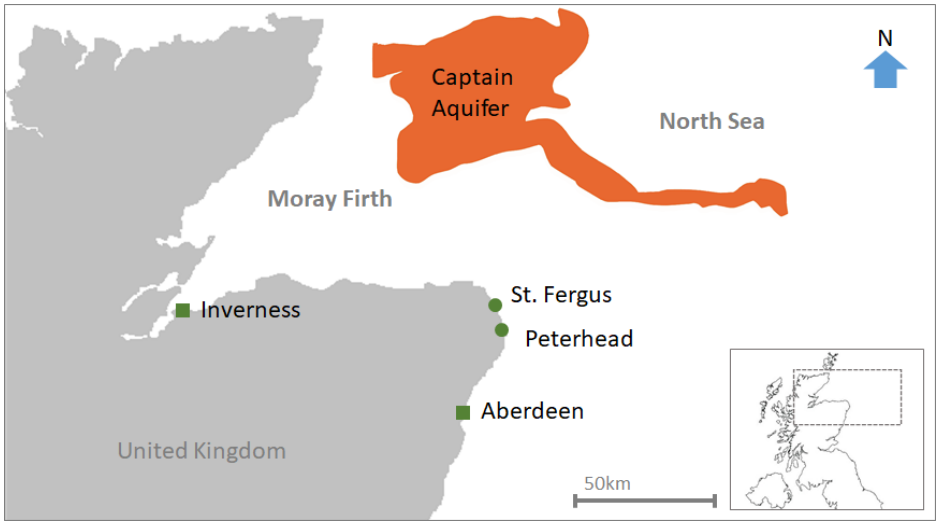

Figure 2: Location of the Captain aquifer in the outer Moray Firth region in the Central North Sea.

Figure 3 shows the formations stratigraphy in the Captain aquifer. The Cretaceous age Captain sandstone provides the main storage interval in Captain aquifer. The Captain sandstone consists of channel-dominated turbidite deposits with generally excellent reservoir properties [28]. The net-to-gross (NTG) ratio is above 75%, with average porosity of 25%. The site shows excellent injectivity with measured core permeability exceeding 1.97 μm^2 (2000 mD) [28].

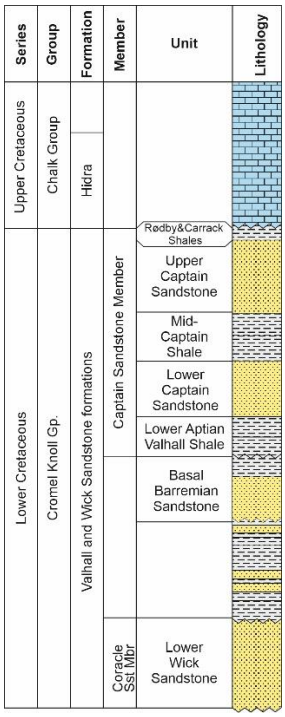

Figure 3: Stratigraphy of formations in the Captain aquifer region, from the Captain Field type well UK 13/22a-7 (modified from [34]).

The storage interval is overlain by the laterally extensive mudstones and shale of the Rodby and Carrack formations which provides excellent seal for many hydrocarbon fields in the region and is expected to provide the necessary seal for CO_2 storage in this aquifer. The base seal is provided by the mudstones of the Lower Valhall Aptain shales [28].

The average Captain Sandstone thickness in the Captain X storage site is approximately 54 m but can reach up to 143 m thick [28]. The mid Captain shale layer splits the Captain sandstone into upper and lower Captain intervals. The upper Captain is a thick, massive, clean and laterally extensive reservoir unit for many hydrocarbon fields within the Captain sand and is expected to be the main storage interval for potential CO_2 storage in Captain aquifer. The lower Captain is a massive medium grained sandstone, laterally restricted and less discontinuous with smaller storage volume than the upper Captain interval [28].

3.2. Captain X Storage Site

The site "X" or the "Captain X" storage site is defined to be a subset or part of the greater Captain aquifer. Captain X covers an area of approximately 344 km^2 or about 10% of the total Captain aquifer area. The site is located in the UKCS quadrants 13 and 14, between the Atlantic and Blake hydrocarbon fields [28]. The corridor shape storage site is limited by pinch out at the north-east and south-west borders while free hydraulic communication can be established at its non-geologically defined, north-west, and south-east boundaries (Figure 4).

The Captain X boundaries have been defined with a two-fold view. First, to avoid the shallower western and the poorer quality eastern parts of the Captain aquifer [28]. Second, to minimise CO_2 storage interaction with other nearby subsurface activities, notably with oil production from the Captain oil field to the north-west, and the potential CO_2 storage programme in the Goldeneye field to the south-east of the storage site (Figure 4) [35]. The Goldeneye field is abandoned and has been previously considered for CO_2 storage developments by Shell [37].

Figure 4: Captain X geological (no flow - blue) and non-geological (open flow - red) boundaries. Major hydrocarbon fields, within and around, Captain X have been highlighted. Outline of field boundaries were obtained from the OGA [35].

With these boundaries assigned, the Captain X site covers the entire abandoned Cromarty field, part of the Blake field to the north-west and the majority of Atlantic field to the south-east (Figure 4). Atlantic and Cromarty are gas condensate fields and have been abandoned since 2009, after less than four years of production each, whereas, Blake is still producing, with production expected to stop after CO_2 injection in Captain X is underway. Although, Atlantic and Cromarty fields have already been abandoned, they still contain unrecovered volumes of hydrocarbon gas left after abandonment.

The Captain aquifer within the boundaries of Captain X is tilted 1-2°, shallower from south-east to north-west. At the Captain X site, the top of the sandstone ranges from 1485 m TVDSS at the crest of the Blake field down to 1980 m TVDSS between Atlantic and Cromarty fields, the location of which is being considered for CO_2 injection [28]. This implies the direction of plume migration will be from south-east toward north-west. The challenge for CO_2 storage development in this site is to contain the plume before crossing the north-west boundary. Given the excellent reservoir properties of Captain sandstone, this migration will probably occur rapidly, and its characteristics will strongly influence the volume of CO_2 that can be safely contained in Captain X. During plume migration, the mixing of the injected CO_2 and the *in-situ* hydrocarbon gas left in Atlantic and Cromarty fields may occur, this

may influence CO_2 storage characteristics in Captain X. We use numerical modelling to investigate this impact in the next section.

4. Materials and Methods

For this numerical analysis, we use the darcy-based Captain Fairway numerical model, constructed previously as part of the ETI-UKSAP study to investigate CO_2 storage in Captain X [28]. Table 1 shows major ETI-UKSAP model parameters. An overview of the model properties and its construction history are provided in the Section 4.1. The full details of the ETI-UKSAP Captain fairway static and dynamic model's construction are described in the ETI report [28]. The original ETI-UKSAP model will be modified in this study to enable correct replication of the physics of the mixing phenomenon. This will be outlined in Section 4.2.

Category	Parameter		Value
Initial condition	Initial pressure at datum (MPa)		19.70 at 1890 m TVDSS
	Temperature (°C)		65
	Brine salinity (mg/L)		56,600
Petrophysical properties	Porosity		0.20
	Average horizontal permeability (μm^2)		0.94 (955 mD)
	Average vertical permeability (μm^2)		0.48 (484 mD)
Water-gas relative permeability (drainage, imbibition)	n_g		3, 3
	n_w		2, 2
	k_{rw} at S_{GR}		1.00, 0.40
	k_{rg} at S_{WR}		0.92, 0.92
	S_{WR}		0.30, 0.30
	S_{GR}		0, 0.29
Rock properties	Rock compressibility (1/MPa)		5.1×10^{-5} at 19.70 MPa
	Rock fracture gradient (kPa/m)		14.80
Fluid properties (at reference initial conditions)	Densities (kg/m^3)	CO_2	645
		A&C* hydrocarbon gas	380
		Blake oil	915
	Viscosities (mPa·s)	CO_2	0.05
		A&C* hydrocarbon gas	0.02
		Blake oil	3.90
Grid parameters	Dimensions of the model		228×112×30
	Areal size of grid blocks (m^2)		400×400
	Average grid blocks thickness (m)		2.6
	Number of active grid blocks		116,130

Table 1: Main Captain fairway numerical model parameters [28]. (*Atlantic and Cromarty).

4.1. Overview of the ETI-UKSAP Conceptual Model

Geometry and extent of the model: Figure 5 shows map (left) and cross-sectional (right) views of the ETI-UKSAP conceptual numerical model. The cross-sectional view (right) is generated along the middle of the numerical model. The model extends over an area larger than the proposed Captain X Site (Figure 4), this is to monitor plume migration and containment post-injection cessation. As the storage site model only partially encompasses the Captain aquifer, numerical aquifers were connected to either end of the storage site, this is to allow pressure dissipation into the greater Captain aquifer as CO_2 is injected into the model.

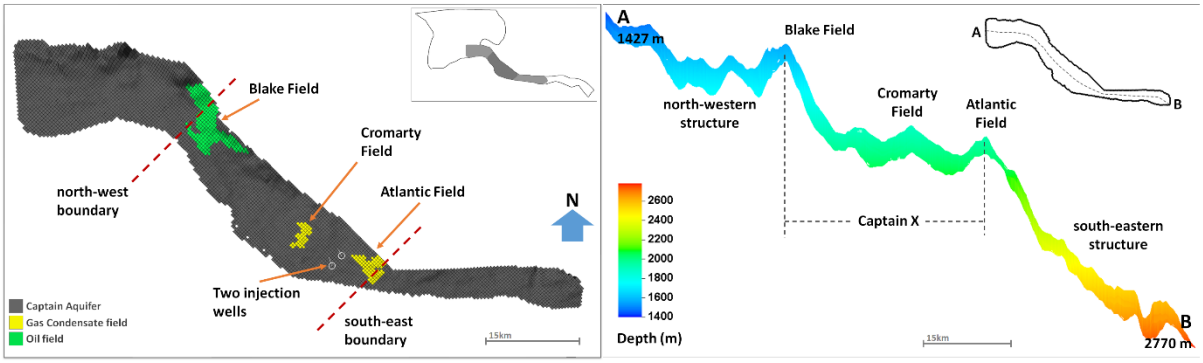

Figure 5: Left: Map view of the ETI-UKSAP numerical model along with the positions of the Blake and abandoned Atlantic and Cromarty fields. The numerical model corresponds with the grey region of the storage site within the Captain aquifer. Right: Cross-section of the numerical model across the dashed (A-B) line [28].

As per the stratigraphy described in Figure 3, the model was constructed between the top and base Captain horizons, and includes both the Upper and Lower Captain Sandstone members separated by the mid-Captain shale layer. The model is assumed to be overlaid and underlaid by no-flow boundaries, as such pressure dissipation into the overburden and underburden was not considered. The numerical model is an upscaled version of the static model built over the area using information from 16 wells, of which 7 were cored, and seismic interpretation available in the area. The static model was built with a rotation of 135° and cell sizes of 200m × 200m in the major horizontal directions. Porosity was modelled using the available interpreted porosity logs whereas permeability was modelled using the available measured core data correlated to the modelled porosity. Schlumberger Petrel was used to build the static model [37] in the ETI-UKSAP study.

Model Upscaling: the upscaling methodology and the size of grids blocks chosen for the numerical simulation could have an important impact on the accuracy of the modelling results, e.g. in the estimated storage capacity or the accurate location of the plume as it migrates. A greater degree of upscaling increases numerical dispersion in the model, which may overestimate CO_2 dissolution and may affect the accuracy of results [38].

The upscaling process in Captain aquifer is not expected to be a great challenge since the main storage interval (upper Captain) is very clean with minimal heterogeneity. Most of the injected CO_2 is also expected to be stored in the upper Captain interval, with little contribution to storage from the lower intervals. In the ETI-UKSAP project, the upscaling process was undertaken to generate a dynamic model able to run many different simulation scenarios in a reasonable time frame. Laterally, the grid was coarsened by a factor of 2, resulting in static model grid blocks coarsened to 400m × 400m to be adapted for the numerical simulation. Vertically, the grid was coarsened by nearly five times, i.e. from 157 layers to 30 accordingly. Vertical upscaling honoured the zonation applied in the static model, while different degrees of coarsening were applied to each zonation. The upscaling reduced the number of cells from around 16.1 million grid blocks in the static model to approximately 116,130 grid blocks in the numerical model. Properties were upscaled following by conventional standard hydrocarbon industry upscaling methods. Porosity was upscaled using the volume weighted arithmetic average method. Horizontal and vertical permeabilities were upscaled using the Cardwell Parsons directional averaging method [40]. Additional information with regard the upscaling procedure of the ETI-UKSAP model can be found in the ETI report [28].

Initialisation, fluid model and displacement parameters: The numerical model is an isothermal model, with the structure initially filled with brine, except for the hydrocarbon fields included in the model, i.e. the Atlantic, Cromarty and Blake fields. Other hydrocarbon fields, beyond the Captain X boundaries, i.e. the Goldeneye gas condensate field to the south-east and the Captain heavy oil field to the north-west (Figure 4), were not included in the model.

A black oil modelling approach was used in the ETI-UKSAP model to account for brine and CO_2 properties and their mutual interactions. The Atlantic and Cromarty fields were populated with estimated post-abandonment hydrocarbon gas volumes. The black oil modelling strategy did not, however, consider mixing in the ETI-UKSAP study, as the CO_2-rich plume migrates and enters into

the abandoned hydrocarbon fields. Instead the emphasis was to first, account for the Atlantic and Cromarty's volume that is not directly available for CO_2 storage as it is already occupied by hydrocarbon gas and second, to take into account the compressibility effect of remained hydrocarbon gas on CO_2 storage characteristics in Captain X. The pressure footprint due to prolonged oil production from the Blake field was also included in the ETI-UKSAP model with matched water withdrawal from this field.

The displacement of CO_2 and water-rich phases in the storage site are controlled by the relative permeability parameters. As no experimental CO_2-water relative permeability measurements are available for the storage site, a Corey-type relative permeability model [41] estimates CO_2 and water relative permeability in the model with parameters as shown in Table 1 [42]. The CO_2-water relative permeability model was based on Shell's results for CO_2 storage modelling in the Captain Sandstone member within the Goldeneye field of the Captain aquifer [42]. Separate drainage and imbibition relative permeability curves were considered in the model development allowing for residual trapping of the plume upon water encroachment with maximum residual gas trapping of S_{GR}=0.29.

Calibration Process: The Captain aquifer is an injection site for which there is no history of CO_2 injection to match or calibrate the model. The calibration process is therefore based on the best available information that could be collected for the site, mainly from the nearby hydrocarbon fields, at this stage of storage development.

The calibration approach was not intended, however, to achieve a detailed well-by-well calibration. Instead, the model pressure was broadly matched with that observed from the Repeat Formation Tests (RFT) measurements in the storage site, the available pressure data from the Blake field and records of fluid withdrawal from the vicinity of the Atlantic and Cromarty structures. In that regard, the size of connected aquifers to the either ends of the model and the transmissibility across the mid-Captain shale were identified as the key subsurface uncertainties for the calibration process, as such they were varied to obtain a reasonable match with the available RFT data. A very low, nonzero, transmissibility across the shale layer was required to achieve an RFT match. Revisiting the calibration process in the future as additional data, including the performance of CO_2 injection in the site, become available is recommended.

Major Identified Uncertainties: Several important uncertainties related to the modelling construction were identified in the ETI-UKSAP modelling study [28]. These include the topology of the top Captain sandstone, the size of connected aquifers, transmissibility across the Captain shale layer, the connectivity to the underburden lower Valhall formation, the considered fracture pressure gradient, and the choice of relative permeability model.

The results of a sensitivity analysis carried out as part of the ETI-UKSAP modelling study indicate that for a pressure restricted injection scenario, in that injection becomes limited exclusively by the pressure footprint, all these uncertainties could be significant to varying degrees. The impact of the identified uncertainties could be significantly different if the storage is considered to become constrained by "plume migration" instead of "pressure footprint".

CO_2 storage development plan: CO_2 storage development plan in the ETI-UKSAP modelling study calls for injecting CO_2 using twin injectors, each injecting at 1.5 MT/year (total 3 MT/year). Injectors are located between the Atlantic and Cromarty fields, at the bottom of the site and some 30 km away from the north-west boundary (Figure 5-left). The philosophy for this injector placement was to maximise the storage efficiency by creating a tortuous path as possible for the injected CO_2 as it migrates to shallower depths, taking maximum advantage of structural, residual and solubility trapping. Injection is carried out only in the upper sand as the lower sands are less extensive which may result in a more rapid pressure build up at the seal-store boundary during CO_2 injection.

The definition of maximum storage capacity in Captain X, as an exemplar open saline aquifer system, mandates that all injected CO_2 is to be contained within the storage boundaries for at least 1,000 years post-injection, with final plume migration velocity smaller than 10m/year [12]. In this regard, the ultimate storage capacity depends just as much on the engineering considerations of CO_2 development as it does on site physical characteristics [14]. Assessing the storage capacity therefore requires a "trial and error" approach, in that the inventory of CO_2 should be varied from an initial estimation until the entire plume is successfully contained with the predefined storage boundaries. Subject to this

definition and with the chosen CO_2 injection engineering, the ETI-UKSAP study concluded a final safe CO_2 storage capacity of 60 MT in the Captain X. As such, CO_2 injection could be sustained using the twin injectors for a maximum duration of 20 years to allow for 1000 years plume containment post injection cessation. In that analysis, however, the impact of CO_2 mixing with remaining hydrocarbon gas in the abandoned Atlantic and Cromarty fields were not considered. Our modelling study takes on this and illustrates how mixing may affect storage characteristics in Captain X.

4.2. Accounting for Mixing in This Study

To properly capture the physics of mixing, it is necessary to account for the variation of plume properties that may occur as non-CO_2 gases are introduced and mixed in the CO_2-rich plume. The black oil modelling approach used in ETI-UKSAP modelling study is unable to simulate this phenomenon since it does not allow the definition of a multicomponent gas phase, a key feature required to capture mixing. To achieve this, the ETI-UKSAP model was adapted into a new compositional fluid description in this study. Opposite to a black oil modelling approach, a compositional Equation of State (EoS) based modelling strategy allows the modification of the plume properties based on the fraction and properties of individual components existing in the plume. For our practical problem, this means the compositional simulation allows the injected CO_2 to be properly differentiated from the resident hydrocarbon gas left in Atlantic and Cromarty fields.

We used Schlumberger Eclipse 300 [43] for the compositional modelling undertaken in this study. The details of the constructed compositional fluid model used in the adapted model are depicted in Table 2. The constructed fluid model is a ternary fluid description composed of pure CO_2, a light (C_L) and a heavy (C_H) hydrocarbon component. The CO_2 component is a standard library component, whereas the other two components were defined to replicate light gas and heavy oil existing in the storage area. The properties of the lighter hydrocarbon component (C_L) were adjusted to broadly represent the hydrocarbon gas properties found in the Atlantic and Cromarty fields. The heavier hydrocarbon component (C_H) was introduced to enable representation of the heavy oil found in the Blake field [28]. A 20-80% mixture of light and heavy components represents oil in the Blake field.

Component	**CO_2**	**C_L**	**C_H**
Type	standard	characterised	characterised
M_w	44.01	60.00	90.00
Ω_A	0.4572	0.4572	0.4572
Ω_B	0.0777	0.0388	0.0777
P_c (kPa)	73.8	8.3	42.2
T_c (°K)	304.0	87.9	562.2
V_c (m^3/kg-mole)	0.0941	0.0979	0.6242
$V_{c\ visc}$ (m^3/kg-mole)	0.0170	0.0842	0.3464
Ω	0.225	0.020	0.570
Gas composition in the Atlantic and Cromarty fields (%)	0	100	0
Oil composition in the Blake field (%)	0	12	88
Injected CO_2 (%)	100	0	0

Table 2: Compositional fluid model parameters used in this modelling study. All parameters are described in the Nomenclature. C_L is the light hydrocarbon component and C_H the heavy hydrocarbon component.

The philosophy of this fluid model construction is not to capture the full physics of the entire mixing phenomena, e.g. possible miscibility development between CO_2 and oil in the Blake field should CO_2 enter the structure. Instead, the emphasis was to capture the key effects pertinent to mixing and its impact on plume migration characteristics in Captain X. Any CO_2 entering the Blake field will be structurally trapped in the Blake structure irrespective of the complex, low-scale compositional interactions that may occur. With only three components, the compositional model can capture the

key mixing phenomenon while having acceptable simulation runtimes. This allows the undertaking of many numerical simulations, each of which entails modelling of plume migration 1000 years after injection cessation to understand the maximum storage capacity in Captain X.

CO_2 and brine mutual interaction is an important consideration for CO_2 storage in saline aquifers. In this adapted model, CO_2 dissolution in brine and the subsequent increase in brine density were simulated using the CO2SOL module of Eclipse 300 [43]. The CO2SOL module estimates the CO_2 solubility in brine from the correlations given by Chang, Coats and Nolen [44]. The effect of salt and CO_2 solubility on water properties is calculated using the Ezrokhi's method [45]. It is also implicitly assumed that mixing does not affect the displacement characteristics of the plume, i.e. the migration of the plume is described and governed by the unique relative permeability model already defined and implemented in the model.

5. Simulation Results and Discussion

Adapting the ETI-UKSAP model to consider for mixing, CO_2 was injected into the modified model using the same twin injectors as discussed above (Figure 5-left). We develop this scenario with an initial guess of 60 MT for CO_2 storage capacity in Captain X, similar to that estimated in the ETI-UKSAP study in that CO_2 will be injected into the model for 20 years followed by 1000 years shut-in period to allow plume migration simulation during that period. Tracking plume migration may provide insight into the significance of mixing and how it influences the storage characteristics in Captain X.

5.1. Impact of Mixing on Plume Migration Characteristics

Figure 6 shows plume evolution and migration, before and post-injection cessation. Cross-sectional images have been generated along the plume migration pathway as have been shown in the corresponding map-views. We used (gas) density profiles to describe the extent of the plume as well as to distinguish between the CO_2 and hydrocarbon gas and to describe mixing between them. Significant density contrast exists between CO_2 and hydrocarbon gas, this allows each to be individually tracked in the plume based on their densities. CO_2-rich regions are shown in red in the plume, whereas hydrocarbon gas-rich regions appear in green. Any mixing between them can be distinguished by the intermediate colours shown in the legend.

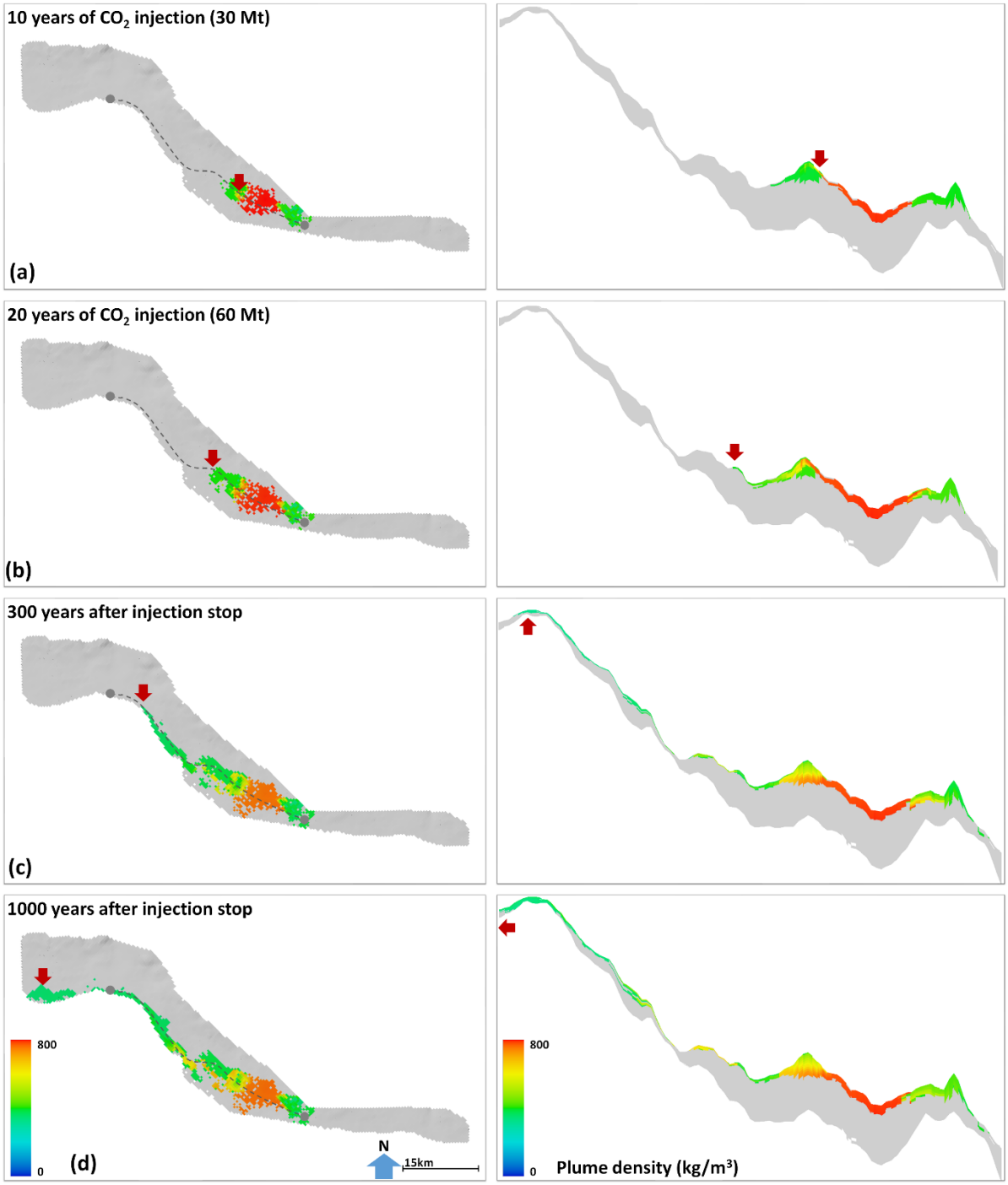

Figure 6: Plume density profiles at several intervals before (a and b) and after (c and d) injection cessation. The edge of the plume has been marked by red arrows. CO_2 and hydrocarbon-rich regions may be identified respectively by red and green colours. Cross-sectional images have been produced along the dashed lines shown in left map-views.

Results show that after 5 years and 15 MT of CO_2 injection, the CO_2 plume arrives at the boundary of the Cromarty field. Since no contact has yet been made between the injected CO_2 and hydrocarbon gas left in Cromarty, the two gases still retain their original properties. Further CO_2 injection causes the CO_2-rich plume to enter the Cromarty structure. The CO_2 plume then begins to mix with the remaining hydrocarbon gas in Cromarty. This mixing reduces the density of CO_2 plume at the leading edge (the developing yellow regions in Figure 6a and later panels). While CO_2 mixes with hydrocarbon at the front, further CO_2 invasion pushes the structurally trapped hydrocarbon gas out of the Cromarty structure. The mixed plume spills out of Cromarty after ~10 years and 30 MT of CO_2 injection (Figure 6a).

It should be noted that the invasion of the CO_2 plume into Cromarty during high pressure CO_2 injection occurs horizontally rather than vertically. This is due to the greater horizontal permeability, in comparison to vertical, and dominance of viscous over buoyancy forces, which supersedes the density contrast between CO_2 and hydrocarbon gas, which otherwise would promote CO_2 sinking upon entry into the Cromarty structure. This can be observed in Figure 6b (cross-sectional) which shows that the edge of CO_2 plume follows the horizontal high permeability path underneath the caprock and does not sink or mix vertically with the remaining hydrocarbon gas in Cromarty. Figure 6b also shows that after 20 years and 60 MT of CO_2 injection, the mobile mixed plume has progressed well beyond the Cromarty structure. Once hydrocarbon gases become mobile and integrate into the plume, the mobile plume is no longer pure CO_2 rather it is a mixture of CO_2 and mobilised hydrocarbon gas, with varying proportions of each gas along the plume. This means the previously immobile hydrocarbon gas, which were otherwise structurally trapped, now became mobile, integrated into the plume, and can migrate with the injected CO_2. This has serious security implications on CO_2 storage in Captain X.

Post injection cessation, the plume's migration velocity decreases but continues to migrate to shallower depths under the influence of buoyancy forces. Plume migration is further promoted by the increased density contrast existing between brine and the mixed plume as the lighter hydrocarbon gases have been mobilised, integrated and mixed into the plume. Figure 6c shows that only 300 years after injection cessation, the leading edge of the plume arrives at the north-west boundary. This is 700 years earlier than envisaged under the storage security requirements, implying that the storage capacity should be smaller than the 60 MT estimated previously [28]. Finally, Figure 6d shows by the end of storage simulation, i.e. 1000 years after CO_2 injection stops, the plume has migrated well beyond the north-west boundary. This suggests that the injected CO_2 inventory should be reduced to accommodate for its proper containment.

As with density profiles (Figure 6), Figure 7 compares CO_2 and hydrocarbon (mole) fractions profiles in the plume at the end of simulation, i.e. 1000 years after injection termination, and highlight the degree of occurred mixing and hydrocarbon mobilisation. Cross sectional images have been produced along the dashed lines shown in the respective map-views. Significant mobilisation of the otherwise structurally trapped Cromarty hydrocarbon gas can be observed in Figure 7, in line with observations made in Figure 6. Interestingly, it can be seen that it is mainly hydrocarbon gas, and not CO_2, that has crossed the north-west storage boundary while the majority of the injected CO_2 became immobilised before reaching the boundary. This is due to the mobilised hydrocarbon gas, from within Cromarty, being pushed immediately ahead of the CO_2 front, causing them to cross the north-west storage boundary well before CO_2.

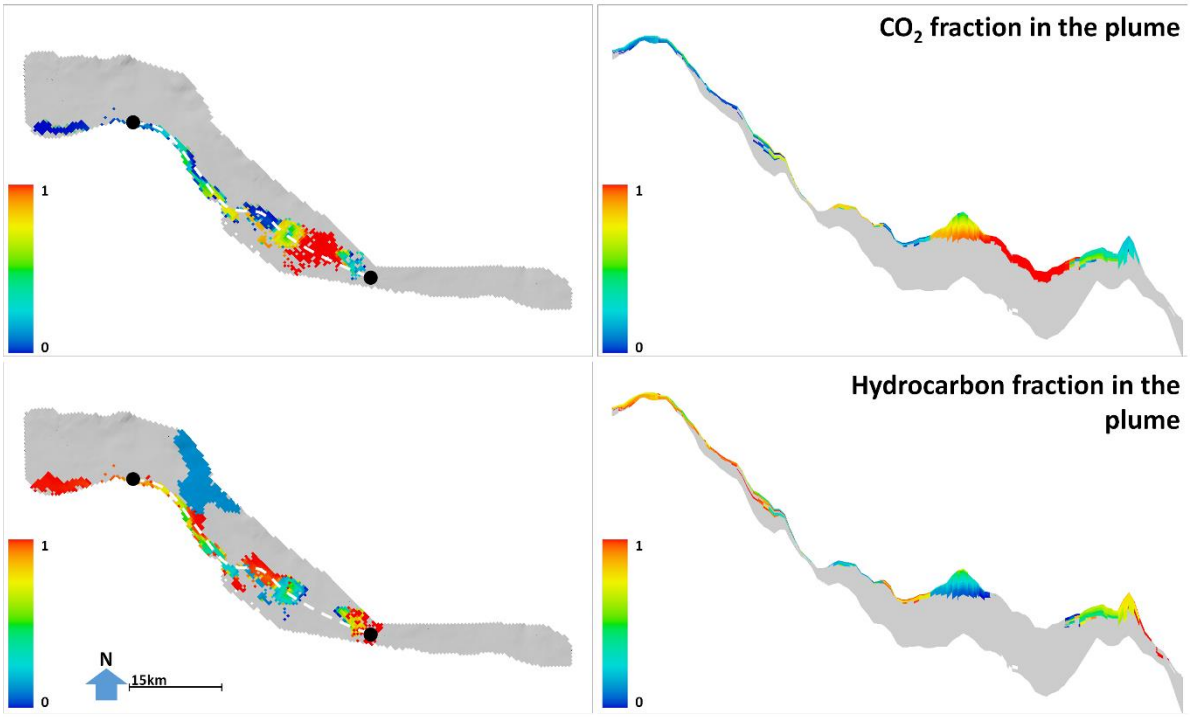

Figure 7: Profiles of CO_2 and hydrocarbon fraction in the plume at the end of simulation (1000 years after injection stop). Cross sectional images have been produced along the dashed lines shown in map-views.

Further inspection of cross-sectional images in Figure 7 shows that long after injection ceases, once buoyancy forces completely dominate, the CO_2 and hydrocarbon gas coexisting in the Cromarty structure segregate due to their considerable density difference; CO_2 sinks below the hydrocarbon gas with minimal exposure to the caprock. Thus, while interaction of CO_2 and hydrocarbons may promote plume migration for the reasons described above, the density contrast between CO_2 and hydrocarbon gas may serve positively to protect the caprock from long-term exposure with CO_2.

In addition to the impact of density contrast shown above, the degree of mixing occurring between CO_2 and hydrocarbon gas is governed by other important physical phenomena such as the mobility ratio between CO_2 and hydrocarbon gas, their molecular diffusion and their mechanical dispersion characteristics. A higher mobility ratio may create a more unstable front between the two gases allowing for larger mixing to occur, although miscibility may retard this induced instability. The great density difference between the two gases may cause one gas to override or underride the other, therefore, limiting the extent of mixing [46].

5.2. Impact of Mixing on CO_2 Storage Capacity and Security in Captain X

The change in the plume properties due to mixing is expected to affect both storage capacity and security in Captain X. The final storage capacity in Captain X is determined by the competition between plume migration, toward the north-west boundary, and the effectiveness of the trapping mechanisms. Mixing negatively promotes plume migration in Captain X, as observed in Figure 6 and Figure 7. Simultaneously, it weakens the effectiveness of trapping mechanisms, particularly the mobilised hydrocarbons are no longer soluble in water and thus, they cannot be immobilised by dissolution in water as it occurs with CO_2. Additionally, CO_2 stripping from the mixed plume as CO_2 selectively dissolves into the aquifer brine makes the plume richer in hydrocarbon fraction and thus, makes it lighter. The combination of these phenomena is expected to reduce CO_2 storage capacity in Captain X.

We use similar definition of storage capacity used in the ETI-UKSAP study as described above. However, we amend the definition in that the plume, which is now mixture of CO_2 and hydrocarbon (and not exclusively injected CO_2), must be contained with Captain X, 1000 years after injection termination. Taking mixing phenomenon into account and under otherwise comparable modelling

conditions between this and the former ETI-UKSAP study, importantly the impact of uncertainties, the ultimate storage capacity in Captain X is found to be 45 MT in this study i.e. 15 MT smaller than estimated previously in the ETI-UKSAP study where mixing was not considered. For this storage capacity, the corresponding storage efficiency was found to be 2.3%. Such a low storage efficiency is characteristic of CO_2 storage in open boundary saline aquifers with low vertical reservoir heterogeneity and large gravity override, which leaves the bulk of the vertical storage column unused [47].

Mixing negatively affects the "storage security" in Captain X as well. Security of storage usually refers to the concept of CO_2 containment in the storage site [5]. However, results illustrated in this study show that in circumstances where mixing mobilises the otherwise structurally trapped hydrocarbon gas, attention must be given to the leakage risk of "both" CO_2 and hydrocarbons. This, consequently, has a critical impact on the risk assessment of such storage projects. Different criteria may be required to define the security of CO_2 storage or different monitoring responses might be needed to distinguish between the leakage of hydrocarbons and CO_2 from the same site. It should be noted that hydrocarbons (e.g. methane) have much greater greenhouse effects than CO_2 should these gases ever reach atmosphere [48].

5.3. Impact of Flow Modelling Uncertainties on the Observed Results

The results demonstrated in this modelling study e.g. the estimated storage capacity and the profiles of plume migration observed in Figure 6 and Figure 7 are affected by several important uncertainties, both of physical and numerical nature.

The physical uncertainties are mostly inherited from the model construction stage and the fact that there is no history of CO_2 injection to calibrate the model with. While properties can be better estimated near the hydrocarbon fields, substantial uncertainty exists away from these structures. Input petrophysical parameters carry substantial uncertainty, particularly away from wells. The topology of the top Captain sandstone is also a significant factor controlling the plume migration profile, the magnitude of structural trapping and the ultimate storage capacity in this site. Substantial uncertainty exists with this regard, as the upper Captain horizon is seismically transparent, making interpretation difficult, particularly away from the hydrocarbon fields [28]. Additional data collection as part of the MMV (Monitoring, Measurement and Verification) programme may enable reduction of this uncertainty in future studies. The volume and properties of the trapped hydrocarbon gas can also affect the degree of mixing. The impact of these uncertainties will be discussed separately in Section 6.

Relative permeability controls the displacement characteristics and the mobility of the plume and simultaneously defines the degree of residual trapping by which the plume can be immobilised. A more mobile plume predicted by the choice of endpoint relative permeability parameters (k_{rg}) can migrate more easily under the influence of gravity, which ultimately reduces the storage capacity to allow for plume containment. Conversely, a higher residual gas saturation (S_{GR}), defined by the relative permeability model, allows larger fraction of plume to be immobilised by residual trapping which could increase the storage capacity. Additionally, whether the chosen relative permeability model can be applied to the entire storage area, which spans over a large region, is another significant uncertainty to be addressed for this modelling study.

Results of modelling can also be affected by the numerical artefacts, i.e. the spatial and temporal discretisation applied to the numerical model. For example, larger grid blocks may increase the artificial numerical dispersion within the model, causing overestimation of CO_2 solubility. This may affect the accuracy of results and the estimated storage capacity. Nevertheless, the discretisation applied in the numerical modelling performed in this study allows mixing to be effectively captured and analysed.

5.4. Impact of Informed Injector Placement to Control the Significance of Mixing

Mitigation of the extensive mixing observed in the above analysis can be achieved through the relocation of the CO_2 injection points. This could divert the migration path of the CO_2-rich plume

away from Cromarty and reduce CO_2-hydrocarbon gas mixing considerably. This, however, depends on sufficient understanding of the geological features controlling the plume migration characteristics. To investigate this, Figure 8 compares the impact of three different injector placement scenarios on the significance of mixing. The base case scenario demonstrated in Figure 6 is also included for comparison as well. Figure 8 illustrates profiles of hydrocarbon fraction in the plume 1000 years after injection cessation. All scenarios simulate the injection of 60 MT of CO_2 using twin injectors positioned differently than the base case model. The severity of mixing can be inferred in each scenario by comparing the extent and the colour of the profiles. The redder the profile indicates a greater fraction of hydrocarbon mobilisation and mixing accordingly.

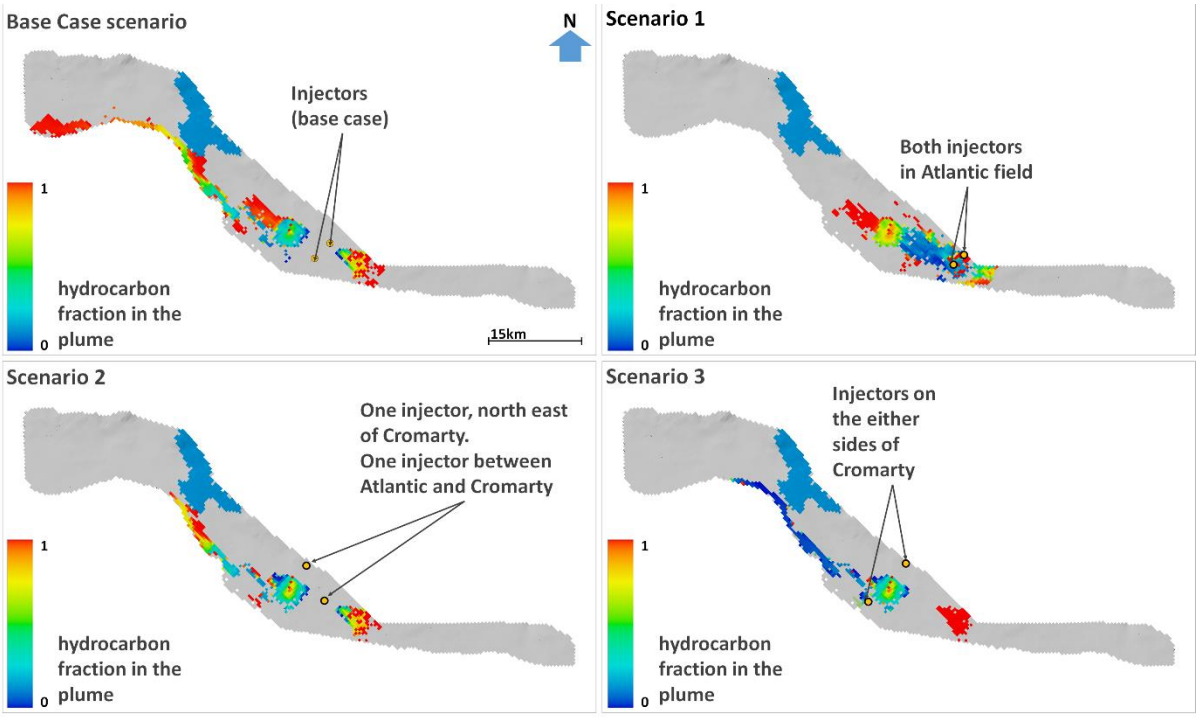

Figure 8: Impact of alternate injector placement to manage the mixing effect. The severity of mixing is significantly dependent on the choice of the injector's locations. Minimum mixing occurs in the third injector placement scenario.

Significant hydrocarbon mobilisation can be observed in the first scenario where injectors are placed directly in the Atlantic field. This illustrates that placing injectors deliberately in depleted hydrocarbon fields to take advantage of the structure traps may result in severe mixing, with potential negative effects as discussed. The second injector placement scenario still shows considerable mixing due to the topology of the geological structure, which promotes the injected CO_2 to divert toward the Cromarty. The third scenario, showing the least degree of mixing, has the injectors placed on either side of Cromarty. This configuration allows the injected CO_2 to migrate to shallower depths with minimum interaction with the hydrocarbon gas left in Cromarty. Results show that part of the injected CO_2 still enters the Cromarty, though the invading volume is not enough to severely trigger mixing. These findings were directly applied for CO_2 storage development plan in Captain X which will be described in Section 7.

5.5. The Choice of Simulator to Capture Mixing

Results of this study also highlight the significance of the modelling strategy on correctly understanding the mixing process and its impact on storage characteristics. Figure 9 compares the degree of plume mobility and migration between compositional and black oil modelling approaches under comparable conditions. This comparison is performed by measuring the distance between the edge of the plume, as it migrates towards the north-west boundary, and the injection point in Captain X. The red line illustrates the distance to the north-west boundary from the injection point; ideally, the

plume must become fully immobilised before reaching this boundary, as mandated by the storage requirement in Captain X and as observed in the above analysis.

Figure 9 shows that the leading edge of the plume is always ahead for the compositional, mixing enabled, model compared to the equivalent black oil model, where mixing has not been considered. In other words, a more mobile plume is always predicted using the compositional model. The difference in plume mobility between the two models is very small immediately post injection cessation, as both models predict an initial maximum plume migration of approximately 10 km from the injection site. However, the extent of plume migration progressively diverges as times go on between the models as, the plume continues to migrate under the influence of gravity. The effect of buoyancy forces is better accounted for in the compositional model as hydrocarbon gas is mixed and carried in the plume. Finally, while the mixing-enabled compositional model predicts plume arrival at the north-west boundary after 300 years (as discussed in Figure 6c), the black oil model predicts this to occur after 1000 years.

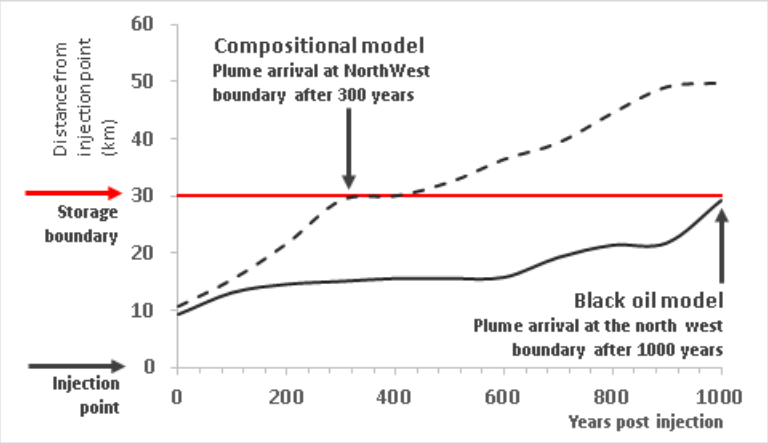

Figure 9: Distance to the leading edge of the plume measured from the injection site; comparison between compositional (with mixing – dashed profile) and black oil (without mixing -solid profile) modelling approaches. Red line marks the distance between injection site and the north-west storage boundary.

A black oil model may be simpler and more convenient, in regards to requiring less computational time and power than a compositional model, to assess the storage capacity. Assuming supercritical CO_2 and liquid water can be represented, respectively, by distinct phases in a black oil model, their properties and their mutual interactions can be correctly replicated at the phase level [49]. However, this modelling approach is unable to consider the impact of composition on phase's properties as properties in a black oil model are defined only at the "phase" level and not at "component" level. A compositional simulation, on the other hand, allows properties to be defined correctly at the component level, a required feature when the impact of mixing is significant. Nevertheless, the use of black oil simulation in the modelling of CO_2 storage processes with mixing phenomenon is only permitted when the properties of the injected CO_2 and the *in-situ* hydrocarbon gas are similar, in that mixing between them does not alter plume properties significantly.

6. Uncertainty in Estimating the Significance of Mixing

Understanding the severity of mixing and its impact on storage characteristics depends on the correct comprehension of the key processes controlling the significance of this phenomenon, some of which may bear considerable uncertainty. In that regard, the primary uncertainties pertinent to mixing could be:

- The volume and properties of any non-CO_2 hydrocarbon gas remaining in the storage site in the abandoned structures,
- The displacement characteristics of non-CO_2 hydrocarbon gas relative to CO_2,
- CO_2-rich plume migration toward hydrocarbon gas accumulations controlled by the formation topology,

A discussion relevant to each item is provided in the below sections.

6.1. The Volume and Properties of the Remaining Non-CO_2 Gases in the Abandoned Structures

The estimated Captain X scenario's storage capacity of 45 MT, in the above analysis, is based on a calculation involving certain volumes and properties of hydrocarbon gas left in Atlantic and Cromarty fields. Should either of these vary, the impact of mixing on the Captain X's storage capacity will change accordingly.

The volume of hydrocarbon gases remaining in the abandoned field structures can affect the final storage capacity in Captain X in two ways: firstly, it directly controls the storage volume which is accessible for CO_2 storage, in that this volume could have been occupied by CO_2 instead of the non-CO_2 gas; secondly, the volume of the remaining hydrocarbon gas controls the degree of mixing, in that the larger the volume of the non-hydrocarbon gases, the larger its impact on the plume properties and migration characteristics upon mixing. While the impact of the former could be linear on the storage capacity in Captain X, the latter may have a non-linear relationship. A sensitivity analysis with regards to the volume of the hydrocarbon gas left in the Cromarty field was undertaken to understand its impact on the storage capacity calculation. Results illustrated in Figure 10 show that if the remaining volume of hydrocarbon gas in Cromarty is reduced by 50% and 100% compared to the base case model (the latter representing no hydrocarbon gas left in the Cromarty field), the corresponding storage capacities will increase to 63 MT and 96 MT, respectively. This represents additional 18 MT and 51 MT increase in the ultimate storage capacity compared to the 45 MT base case model discussed above. The results also show that there is a negative nonlinear dependency between the volume of remaining hydrocarbon gas in the Cromarty field and the ultimate storage capacity observed in Captain X. In other words, more CO_2 can be stored in Captain X relative to the volume of Cromarty hydrocarbon gas that has been removed from the system. This nonlinear dependency can be attributed to the elimination of the mixing effect.

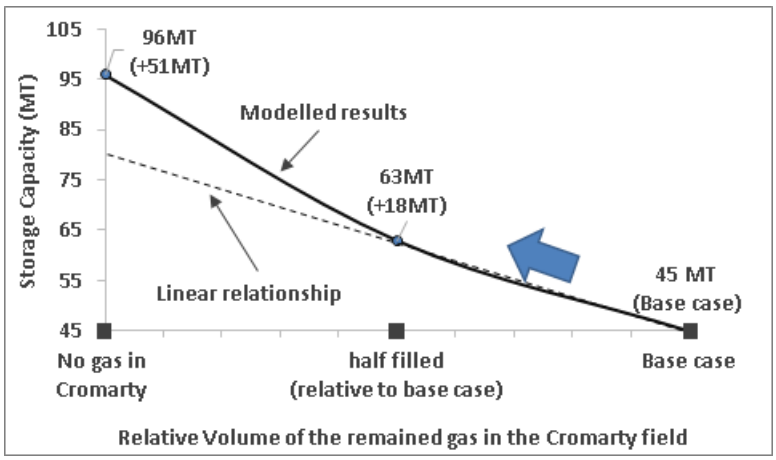

Figure 10: Sensitivity of the maximum CO_2 storage capacity in Captain X with regard the assumed "volume" of hydrocarbon gas remained in Cromarty after its abandonment.

The properties of hydrocarbon gas can also affect the significance of mixing and storage capacity in Captain X. A lighter assumed hydrocarbon gas can affect the density and migration characteristics of the CO_2-rich plume more significantly. Figure 11 shows how storage capacity may vary in the Captain X as the density of the hydrocarbon gas assumed to be left in Cromarty is varied relative the assumed base case scenario (45 MT). It can be seen that an increase or decreases of hydrocarbon gas density correlates with smaller or larger storage capacities in Captain X.

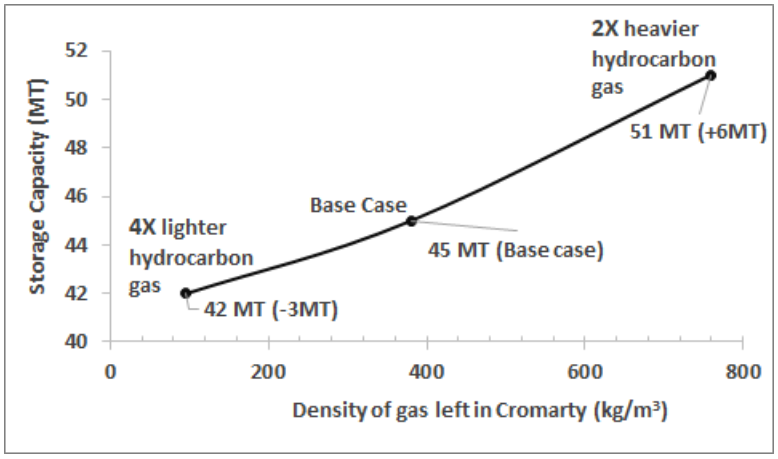

Figure 11: Sensitivity of the maximum CO_2 storage capacity in Captain X with regard the assumed "density" of hydrocarbon gas remained in Cromarty after its abandonment.

While significant uncertainty may exist with regard the estimation of the remaining volumes of non-CO_2 gases existing in the storage site prior to CO_2 storage, the uncertainty regarding the properties of such non-CO_2 gases are expected to be relatively small. This due to the hydrocarbon gas having been actually produced to the surface, which means their properties should have been measured with a high degree of confidence.

6.2. Displacement Characteristics of Non-CO_2 Gases

The displacement characteristics of a plume (described by relative permeability) may change as CO_2 mixes with non-CO_2 gases existing in the storage site. The current understanding of mixing and its impacts on the storage characteristics in Captain X assume that mixing of CO_2 and hydrocarbon gases does not alter the capillary entry pressures and relative permeability characteristics of the plume. In other words, the displacement of plume, once hydrocarbon gases are mixed and carried with CO_2, is still described with the same relative permeability model as for pure CO_2 irrespective of the composition of the plume. In reality, however, mixing may alter the relative permeability characteristics in particular the effectiveness of the residual trapping acting on the plume [50]. This is an important consideration which needs additional investigation in future studies.

6.3. Uncertainty in Site Topography

The topography of the reservoir controls the plume migration characteristics and is vital in determining the ultimate storage capacity in an open boundary saline aquifer. Estimating the impact of mixing on the storage capacity and security in Captain X relies heavily on the correct prediction of the plume migration profile from the injection point toward the non-CO_2 gases accumulation. In Captain X, significant uncertainty exists with regard the storage site topology, as discussed previously, and the current comprehension of mixing is based on model topology inferred through seismic interpretation process. Should it be changed, the significance of mixing will change accordingly.

7. Applying the Findings to CO_2 Storage Development in Captain X

The findings of this study were successfully applied to the CO_2 storage development plan in the Captain X site [51]. Given the importance of mixing, the recommended CO_2 storage design in the Captain X calls for the use of four injectors with accurate CO_2 injection inventories allocated for each injector (Figure 12). Two of the four injectors should be located between the Atlantic and Cromarty fields (G1 and G2). These injectors target the storage volume between the Atlantic and Cromarty fields, with the injection inventories, carefully adjusted to minimise the possibility of CO_2 entering into these fields. The other two injectors should be placed on either side of the Cromarty field, allowing the periphery of the Cromarty field to be targeted all the way up to the north-west boundary, without CO_2 interfering with the remaining hydrocarbon gas in the Cromarty field. Part of the injected

CO_2 migrates and dissolves in the remaining oil in the Blake field, though this happens well after the expected abandonment of Blake. With this arrangement of injectors, Figure 12 shows the final plume profiles, 1,000 years post-injection; almost 92.1 MT of CO_2 can be safely stored within the Captain X boundaries without triggering the mixing phenomenon.

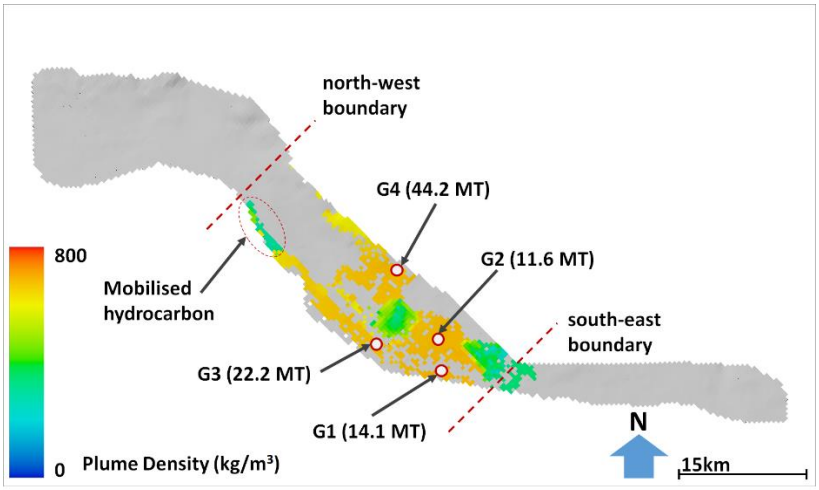

Figure 12: Density profile showing the final plume distribution, 1000 years post-injection for CO_2 storage development in Captain X. Mixing was carefully managed by informed placement of injectors and accurate allocation of CO_2 inventory to each injector.

As with Figure 6, a density profile has been used in Figure 12 to distinguish between CO_2 and resident hydrocarbon gas in the Atlantic and Cromarty fields and indicate the degree of mixing between them. Compared to Figure 6d, which shows profiles 1000 years post injection, it can be seen that mixing has been largely managed and eliminated in Figure 12. Mobilised hydrocarbon gas can only be observed in a small section of the plume as shown, nevertheless, the entire plume is completely contained within the boundaries of Captain X, 1000 years after injection cessation.

8. Conclusions

This study shows that mixing between injected CO_2 and trapped hydrocarbon gas within the storage site has significant impact on the storage capacity and security, in the Captain X open saline aquifer system. If not properly handled, mixing may reduce the storage capacity by promoting buoyancy effects between the plume and the formation brine causing faster plume migration. This leads to earlier than expected CO_2 breakthrough from the store's non-geologically set boundary, which can only be rectified by reducing the injected CO_2 inventory. Excessive mixing may also compromise the storage security as it mobilises the previously immobile hydrocarbon gas out of the hydrocarbon trapping structures. Consequently, in such scenarios the leakage risk is more complex, and attention must be given to the leakage risk of "both" CO_2 and hydrocarbon gas and not exclusively CO_2. The choice of the modelling strategy is vital in providing a correct understanding of the mixing effect and its impact on the storage characteristics. The use of a black oil modelling approach in scenarios where mixing phenomenon is likely could be misleading. In such a circumstance a compositional modelling approach must be employed.

Mixing can be reduced by careful injector placement and careful allocation of CO_2 inventory for each of the injection wells to minimise interaction of CO_2 with hydrocarbon gas during plume migration. The severity of mixing is dependent on the volume and the properties of the remaining hydrocarbon gas in the abandoned storage site. The more hydrocarbon gas left in an abandoned field in the storage site, the greater will be the impact of mixing on plume migration. Similarly, the lighter these non-CO_2 gases, the greater the negative effect.

While this study enhances understanding of the concept of mixing and its impact on CO_2 storage characteristics in open saline aquifers, the findings should not discourage operators from deploying CO_2 storage into such aquifer systems hosting depleted hydrocarbon reservoirs. Rather, the focus of this analysis is to place emphasis on having correct understanding of the mixing phenomenon and a

clear strategy on how to deal with it. The findings of this study were successfully implemented and applied in the CO_2 design process in Captain X, leading to enhance understanding of the storage characteristics and an injection design that reduces the risk of mixing in the storage complex. As with Captain aquifer in the North Sea (UK), the lessons learnt in this analysis are expected to be applicable to saline aquifers located in other storage provinces, such as the wider North Sea region (Europe), the Gulf of Mexico (United States) or the Pearl River Mouth Basin (China). Many of these provinces host petroleum systems and such mixing could be an important consideration for CO_2 storage in these targets.

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References

[1] Goldthau A, Westphal K. Why the Global Energy Transition Does Not Mean the End of the Petrostate. Global Policy 2019;10(2):279-83. https://doi.org/10.1111/1758-5899.12649

[2] Johnsson F, Kjärstad J and Rootzén J. The threat to climate change mitigation posed by the abundance of fossil fuels. Climate policy 2019;19(2): 258-74. https://doi.org/10.1080/14693062.2018.1483885

[3] Kolster C, Masnadi MS, Krevor S, Mac Dowell N, Brandt AR. CO2 enhanced oil recovery: a catalyst for gigatonne-scale carbon capture and storage deployment? Energy & Environmental Science 2017; 10(12): 2594-2608. https://doi.org/10.1039/C7EE02102J

[4] UK government (GOV.UK). UK becomes first major economy to pass net zero emissions law, https://www.gov.uk/government/news/uk-becomes-first-major-economy-to-pass-net-zero-emissions-law; 2019 [accessed 20 July 2020].

[5] Alcalde J, Flude S, Wilkinson M, Johnson G, Edlmann K, Bond CE et al. Estimating geological CO_2 storage security to deliver on climate mitigation. Nature communications 2018;9(1):2201. https://doi.org/10.1038/s41467-018-04423-1

[6] Akhurst M, Callaghan E, Hannis S, Kirk K, Monaghan A, Pearce J et al. Optimising CO_2 storage in geological formations; a case study offshore Scotland. SCCS 2015. Available from: https://www.sccs.org.uk/images/expertise/reports/co2multistore/SCCS-CO2-MULTISTORE-Report.pdf [accessed 20 July 2020].

[7] Niemi A, Bear J, Bensabat J. Geological storage of CO_2 in deep saline formations. Dordrecht, Netherlands: Springer; 2017. https://doi.org/10.1007/978-94-024-0996-3

[8] Bentham M, Mallows T, Lowndes J, Green A. CO_2 Storage Evaluation Database (CO2Stored): the UK's online storage atlas. Energy Procedia 2014;63,5103-13. https://doi.org/10.1016/j.egypro.2014.11.540

[9] Energy Technology Institute. Strategic UK CCS Storage Appraisal, https://www.eti.co.uk/programmes/carbon-capture-storage/strategic-uk-ccs-storage-appraisal; 2019 [accessed 20 July 2020]

[10] Heinemann N, Wilkinson M, Pickup GE, Haszeldine RS, Cutler NA. CO_2 storage in the offshore UK Bunter Sandstone Formation. International Journal of Greenhouse Gas Control 2012; 6:210-19. https://doi.org/10.1016/j.ijggc.2011.11.002

[11] Williams JDO, Jin M, Bentham M, Pickup GE, Hannis SD, Mackay EJ. Modelling carbon dioxide storage within closed structures in the UK Bunter Sandstone Formation. International Journal of Greenhouse Gas Control 2013; 18:38-50. https://doi.org/10.1016/j.ijggc.2013.06.015

[12] Goater AL, Bijeljic B, Blunt MJ. Dipping open aquifers—The effect of top-surface topography and heterogeneity on CO_2 storage efficiency. International Journal of Greenhouse Gas Control 2013; 17:318-31. https://doi.org/10.1016/j.ijggc.2013.04.015

[13] Akhurst M, Mallows T, Pearce J, Mackay E. Assessing interactions between multiple geological CO_2 storage sites to optimize capacity in regionally extensive storage sandstones. Energy Procedia 2017;114:4571-82. https://doi.org/10.1016/j.egypro.2017.03.1577

[14] Celia MA, Bachu S, Nordbotten JM, Bandilla KW. Status of CO_2 storage in deep saline aquifers with emphasis on modelling approaches and practical simulations. Water Resources Research, 2015;51(9):6846-92. https://doi.org/10.1002/2015wr017609

[15] Heinemann N, Stewart RJ, Wilkinson M, Pickup GE, Haszeldine RS. Hydrodynamics in subsurface CO_2 storage: tilted contacts and increased storage security. International Journal of Greenhouse Gas Control 2016; 54:322-29 https://doi.org/10.1016/j.ijggc.2016.10.003

[16] Goater AL, Chadwick RA. Implications of alternative post-injection regulatory guidance upon CO_2 storage in dipping open aquifers. Energy Procedia 2013;37:7756-65. https://doi.org/10.1016/j.egypro.2013.06.722

[17] Ringrose PS, Meckel TA. Maturing global CO_2 storage resources on offshore continental margins to achieve 2DS emissions reductions. Scientific reports 2019;9(1):1-10. https://doi.org/10.1038/s41598-019-54363-z

[18] Sun X, Alcalde J, Gomez-Rivas E, Struth L, Johnson G, Travé A. Appraisal of CO_2 storage potential in compressional hydrocarbon-bearing basins: global assessment and case study in the Sichuan Basin (China). Geoscience Frontiers. 2020: In press. https://doi.org/10.1016/j.gsf.2020.02.008

[19] Meckel TA, Trevino R, Hovorka SD. Offshore CO_2 storage resource assessment of the northern Gulf of Mexico. Energy Procedia 2017; 114:4728-34. https://doi.org/10.1016/j.egypro.2017.03.1609

[20] Agartan E, Gaddipati M, Yip Y, Savage B, Ozgen C. CO_2 storage in depleted oil and gas fields in the Gulf of Mexico. International Journal of Greenhouse Gas Control, 2018;72: 38-48. https://doi.org/10.1016/j.ijggc.2018.02.022

[21] Farzaneh H, McLellan B, Ishihara KN. Toward a CO_2 zero emissions energy system in the Middle East region. International Journal of Green Energy, 2016;13(7):682-94. https://doi.org/10.1080/15435075.2014.889014

[22] Energy Technology Institute. Progressing Development of the UK's Strategic Carbon Dioxide Storage Resource. A Summary of Results from the Strategic UK CO_2. ETI 2016. Available from: https://s3-eu-west-1.amazonaws.com/assets.eti.co.uk/legacyUploads/2016/04/D16-10113ETIS-WP6-Report-Publishable-Summary.pdf [accessed 20 July 2020]

[23] Shell. Peterhead CCS project, Dynamic Reservoir Modelling Report. Doc No: PCCS-05-PT-ZR-3323-00002 2014.

[24] Alcalde J, Heinemann N, Mabon L, Worden RH, deConinck H, Robertson H et al. Acorn: Developing Full-chain Industrial Carbon Capture and Storage in a Resource-and

Infrastructure-Rich Hydrocarbon Province. Journal of Cleaner Production 2019; 223:963-71. https://doi.org/10.1016/j.jclepro.2019.06.087

[25] Oldenburg, C., Webb, S.W., Pruess, K. & Moridis, G.J., 2004. Mixing of stably stratified gases in subsurface reservoirs: A comparison of diffusion models. Transport in Porous Media, 54, 323-34. https://doi.org/10.1023/b:tipm.0000003748.74155.48

[26] Ma J, Li Q, Kempka T, Kühn M. Hydromechanical response and impact of gas mixing behaviour in subsurface CH_4 storage with CO_2-based cushion gas. Energy & Fuels 2019; 33:6527-41. https://doi.org/10.1021/acs.energyfuels.9b00518

[27] Hassanpouryouzband, A, Joonaki E, Edlmann K, Heinemann N, Yang J. Thermodynamic and transport properties of hydrogen containing streams. Nature Scientific Data. 2020;7:222. https://doi.org/10.1038/s41597-020-0568-6

[28] Energy Technology Institute. Captain X Site Storage Development Plan. Strategic UK Storage Appraisal project, D13: WP5D Report. ETI 2016.

[29] Schlumberger. PVTi reference manual. 2014.

[30] Jin M, Mackay EJ, Quinn M, Hitchen K, Akhurst M. Evaluation of the CO_2 storage capacity of the Captain Sandstone Formation. Presented at the SPE Europec/EAGE Annual Conference Copenhagen 2012. https://doi.org/10.2118/154539-ms

[31] Rennie A, Ackhurst MC, Gomersall SD, Pershad H, Todd AC, Forshaw S et al. Opportunities for CO_2 Storage around Scotland; An Integrated Strategic Research Study. Scottish Carbon Capture and Storage. SCCS 2009. Available from: https://www.sccs.org.uk/images/expertise/reports/opportunities-for-co2/CO2-JointStudy-Full.pdf [accessed 20 July 2020]

[32] Ackhurst MC, Gafiera JDL, Hitchen K, Kearsey T, Lawrence DJD, Long D et al. Progressing Scotland's CO_2 storage opportunities. SCCS 2011. Available from: https://era.ed.ac.uk/handle/1842/15726

[33] Allen MJ, Faulkner DR, Worden RH, Rice-Birchall E, Katirtsidis N, Utley JEP. Geomechanical and petrographic assessment of a CO_2 storage site: Application to the Acorn CO_2 Storage Site, offshore United Kingdom. International Journal of Greenhouse Gas Control; 2020, 94, 102923. https://doi.org/10.1016/j.ijggc.2019.102923

[34] Copestake P, Sims AP, Crittenden S, Hamar GP, Ineson JR, Rose PT, et al. Lower Cretaceous. In: Evans, D, Graham, C, Armour, A, and Bathurst, P. The Millennium Atlas: petroleum geology of the central and northern North Sea, London: The Geological Society of London; 2003, p. 191-211.

[35] Peterhead CCS project, Static Models Report. Shell, Doc No:
PCCS-05-PTD-ZG-0580-00001. 2015.

[36] UK Oil and Gas Authority. https://www.ogauthority.co.uk/; 2020 [accessed: 20 July 2020]

[37] Tucker O, Tinios L. Experience in developing the Goldeneye Storage Permit Application. Energy Procedia 2017; 114:7466-79. https://doi.org/10.1016/j.egypro.2017.03.1880

[38] Schlumberger. Petrel manual. 2017.

[39] Green CP, Ennis-King J. Spatial grid correction for short-term numerical simulation results of carbon dioxide dissolution in saline aquifers. Computational Geosciences; 2012, 16(4):1153-61. https://doi.org/10.1007/s10596-012-9309-z

[40] Pyrcz MJ, Deutsch CV. Geostatistical reservoir modelling. Oxford university press; 2014

[41] Lake LW. Enhanced oil recovery: Englewood Cliffs, N.J.: Prentice Hall; 1989

[42] Shell. UK carbon capture and storage demonstration competition. UKCCS-KT-S7.19-Shell-002, SCAL Report. Scottish Power CCS Consortium 2011.

[43] Schlumberger. Eclipse 300 reference manual. 2014.

[44] Chang YB, Coats BK, Nolen JS. A Compositional model for CO_2 floods including CO_2 solubility in water. SPE Reservoir Evaluation & Engineering 1998; 1(2):155-60. https://doi.org/10.2118/35164-pa

[45] Zaytsev ID, Aseyev GG. Properties of Aqueous Solutions of Electrolytes. Boca Raton, Florida: CRC Press; 1992.

[46] Feldmann F, Hagemann B, Ganzer L, Panfilov M. Numerical simulation of hydrodynamic and gas mixing processes in underground hydrogen storages. Environmental Earth Sciences 2016; 75(16):1165. https://doi.org/10.1007/s12665-016-5948-z

[47] Gorecki CD, Sorensen JA, Bremer JM, Knudsen D, Smith SA, Steadman EN et al. A. Development of storage coefficients for determining the effective CO_2 storage resource in deep saline formations. In SPE International Conference on CO_2 Capture, Storage and Utilization 2009. https://doi.org/10.2118/126444-ms

[48] United States Environmental Protection Agency, Understanding Global Warming Potentials; https://www.epa.gov/ghgemissions/understanding-global-warming-potentials. 2019 [accessed 20 July 2020]

[49] Hassanzadeh H, Pooladi-Darvish M, Elsharkawy AM, Keith DW, Leonenko Y. Predicting PVT data for CO_2–brine mixtures for black-oil simulation of CO_2 geological storage. International Journal of Greenhouse Gas Control 2008; 2(1):65-77. https://doi.org/10.1016/s1750-5836(07)00010-2

[50] Honarpour MM, Relative permeability of petroleum reservoirs: CRC press; 2018. https://doi.org/10.1201/9781351076326

[51] ACT-Acorn. D07 Acorn CO_2 Storage Site Development Plan. PBD 2017. Available from: https://actacorn.eu/sites/default/files/ACT%20Acorn%20-%20Acorn%20CO2%20Storage%20Site%20Development%20Plan%201.0_0.pdf [accessed 20 July 2020]

Nomenclature

CCS - Carbon Capture and Storage
MMV - Monitoring, Measurement and Verification
MT - Mega Tonnes
RFT - Repeat Formation Tester
TVDSS - True Vertical Depth SubSea
UKCS - United Kingdom Continental Shelf

M_w - molecular weight
mD - milli-Darcy (equivalent to 9.869×10^{-16} m^2 or 9.869×10^{-4} μm^2)
P_c - Critical pressure
T_c - Critical temperature
V_c - Critical volume
$V_{c\ visc}$ Critical volume for viscosity calculation
ω - Acentric factor
Ω_A - Equation of state parameter (A)
Ω_B - Equation of state parameter (B)
n_g - Corey exponent – gas relative permeability
n_w - Corey exponent – water relative permeability
k_{rw} - End-point water relative permeability
k_{rg} - End-point gas relative permeability
S_{WR} - Irreducible water saturation (drainage), Critical water saturation (imbibition)
S_{GR} - Connate gas saturation (drainage), Irreducible gas saturation (imbibition)